# Parallel netCDF: A High Performance API for NetCDF File Access

#### **Overview**

Parallel netCDF (PnetCDF) is a library providing high-performance I/O while still maintaining file-format compatibility with Unidata's NetCDF.

NetCDF gives scientific programmers a space-efficient and portable means for storing data. However, it does so in a serial manner, making it difficult to achieve high I/O performance. By making some small changes to the NetCDF APIs, PnetCDF can use MPI-IO to achieve high-performance parallel I/O.

- <u>Download</u> has the latest release and development links as well as information about SVN access.
- Documentation: a QuickTutorial, plus papers, presentations, articles, and other resources
- Benchmarking: tools and suggestions for evaluating PnetCDF performance

#### **News**

- 24 September 2012: PnetCDF 1.3.1 released. See ReleaseNotes-1.3.1 for more details.
- A new API ncmpi\_inq\_buffer\_usage/nfmpi\_inq\_buffer\_usage is added for inquiring the current usage of the internal buffer used by the "buffered"-put APIs.
- 26 June 2012: PnetCDF 1.3.0 released. See ReleaseNotes-1.3.0 for more details.
- In the 1.3.0 release, the unsigned and 64-bit integer data types are supported for CDF-5 format. The unsigned data types include NC\_UBYTE, NC\_USHORT, NC\_UINT, and NC\_UINT64. The 64-bit integer data types are NC\_INT64 and NC\_UINT64.
- New APIs for supporting more data types are added. For C, they are ncmpi\_(i)put/(i)get\_var\*\_ushort/uint/longlong/ulonglong. For Fortran, they are nfmpi\_(i)put/(i)get\_var\*\_int8.
- A new set of "buffered"-put APIs is supported in 1.3.0 release. The nonblocking iput/iget APIs require the contents of user buffers not to be changed until the wait call completed. The bput APIs use a user attached buffer to make a copy of request data, so the user buffer is free to change once the bput call returns.
- The special character set, "special2", and multi-byte UTF-8 encoded characters introduced in the CDF-2 file format for variable, dimension, and attribute name strings are now supported.
- A set of example programs and **QuickTutorial** are now available.
- 19 August 2010: PnetCDF 1.2.0 released. See ReleaseNotes-1.2.0 for more details.
- Nonblocking I/O is redesigned in the 1.2.0 release. It defers the I/O requests until "wait" call, so small requests can be aggregated into large ones for better performance.
- Two new hints, nc\_header\_align\_size and nc\_var\_align\_size, are added. The former allows pre-allocation of a larger header size to accommodate new header data in case new variables or attributed are added later. The latter aligns the starting file offsets of non-record variables. Refer to <a href="VariableAlignment">VariableAlignment</a> for a more detailed description.
- Data consistency control has been revised. A more strict consistency can be enforced by using NC\_SHARE mode at the file open/create time. In this mode, the file header is synchronized to the file if its contents have changed. Such file synchronization of calling MPI\_File\_sync() happens in many places, including ncmpi\_enddef(), ncmpi\_redef(), all APIs that change global or variable attributes, dimensions, and number of records.

• As calling MPI\_File\_sync() is very expensive on many file systems, users can choose more relaxed data consistency, i.e. by not using NC\_SHARE. In this case, file header is synchronized among all processes in memories. No MPI\_File\_sync() will be called if header contents have changed.

MPI\_File\_sync() will only be called when switching data mode, i.e

ncmpi\_begin\_indep\_data() and ncmpi\_end\_indep\_data().

## A Note About Large File Support

The <u>CDF</u> (or CDF-1) file format has been in use by NetCDF library through version 3.5.1.

Starting from 3.6.0, the serial NetCDF library added support for <u>CDF-2</u> format. With this format, even 32 bit platforms can create NetCDF files greater than 2GB in size. CDF-2 also allows more special characters in the name strings of defined dimension, variables, and attributes. The support was based largely on work from Greg Sjaardema.

As of PnetCDF 0.9.2, we ship with support for large file size specified in CDF-2 format. See <u>README.large files</u> in the source tree for more information.

Starting from 1.3.0, PnetCDF supports  $\underline{\text{CD-5}}$  file format: adding unsigned and 64-bit integer data types and allowing variables with more than  $2^{32}$  array elements.

#### File and Variable Limits

Both PnetCDF and NetCDF share limitations on file and variable sizes. More information can be found on the <u>FileLimits</u> page.

### **Required Software**

PnetCDF requires an MPI implementation with MPI-IO support. Most MPI libraries have this nowadays. A parallel file system would also go a long way towards achieving highest performance.

## **Related Projects**

PnetCDF makes use of several other technologies.

- <u>ROMIO</u>, an implementation of MPI-IO, provides optimized collective and noncontiguous operations. It also provides an abstract interface for a large number of parallel file systems.
- One of those file systems ROMIO supports is <u>PVFS</u>, a high performance parallel filesystem for linux clusters.

Today, there are several options for high level I/O libraries. Here are some discussions on the role of PnetCDF in this ecosystem:

- pnetcdf\_vs\_hdf5?
- pnetcdf vs netcdf4?

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## **Mailing List**

We discuss the design and use of the PnetCDF library on the parallel-netcdf@mcs.anl.gov mailing list. Anyone interested in developing or using PnetCDF is encouraged to join. Visit the list information page for details.

The URL for the list archive is <a href="http://lists.mcs.anl.gov/pipermail/parallel-netcdf/">http://lists.mcs.anl.gov/pipermail/parallel-netcdf/</a>. You can browse even older mailing list messages at the older mailing list archives

### **Project Members**

- Rob Latham, Rob Ross, and Rajeev Thakur (Argonne National Lab)
- Wei-keng Liao, Seung Woo Son, and Alok Choudhary (Northwestern University)
- Kui Gao (formally postdoc at Northwestern, now Dassault Systèmes Simulia Corp.)
- Jianwei Li (Northwestern, graduated in 2006)
- Bill Gropp (formerly ANL, now UIUC)

#### **Citations**

When referring to the Parallel netCDF project, please use our "permanent" URL: www.mcs.anl.gov/parallel-netcdf. The 'trac' or 'www-unix' URLs could change.

If you are looking for a reference to use in a published paper, please cite our SC2003 paper

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